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# Fluoren-9-one oxime

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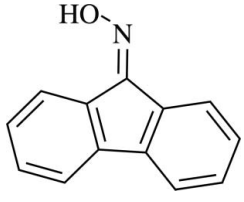
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.029; $wR$ factor = 0.075; data-to-parameter ratio = 13.9.

In the title molecule, $C_{13}H_9NO$, the fluorene system and the oxime group non-H atoms are essentially coplanar, with a maximum deviation from the fluorene mean plane of 0.079 (2) Å for the oxime O atom. A short intramolecular C—H···O generates an $S$(6) ring. In the crystal, molecules related by a twofold screw axis are connected by O—H···N hydrogen bonds, forming [100] chains Within these chains, molecules related by a unit translation along [100] show $\pi$–$\pi$ stacking interactions between their fluorene ring systems with an interplanar distance of 3.347 (2) Å. The dihedral angle between the fluorene units of adjacent molecules along the helix is 88.40 (2)°. There is a short C—H···$\pi$ contact between the fluorene groups belonging to neighbouring chains.

## Related literature

For the original procedure for the preparation of the title compound, see: Moore & Huntress (1927). For the use of the title compound as a starting material for the synthesis of bioactive compounds, see: Amlaiky *et al.* (1983); Ni *et al.* (2009); Rad *et al.* (2012).




## Experimental

### Crystal data

$C_{13}H_9NO$
$M_r$ = 195.21
Orthorhombic, $P2_12_12_1$
$a$ = 4.8009 (1) Å
$b$ = 12.2309 (2) Å
$c$ = 16.0247 (3) Å
$V$ = 940.96 (3) Å$^3$
$Z$ = 4
Cu $K\alpha$ radiation
$\mu$ = 0.70 mm$^{-1}$
$T$ = 100 K
0.16 × 0.13 × 0.13 mm

### Data collection

Agilent SuperNova (Dual, Cu at zero, Atlas) diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2013)
$T_{min}$ = 0.890, $T_{max}$ = 1.000
7588 measured reflections
1942 independent reflections
1865 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.029

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.075
$S$ = 1.05
1942 reflections
140 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.13 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$
Absolute structure: Flack parameter determined using 735 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.16 (13)

**Table 1**
Hydrogen-bond geometry (Å, °).

*Cg*1 is the centroid of the C2–C7 ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C12—H12···O1 | 0.95 | 2.38 | 2.898 (2) | 114 |
| O1—H1···N1$^{i}$ | 0.98 (3) | 1.80 (3) | 2.7758 (18) | 169 (3) |
| C5—H5···*Cg*1$^{ii}$ | 0.95 | 3.08 | 3.873 | 142 |

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, -z+1$; (ii) $x-\frac{1}{2}, -y+\frac{1}{2}, -z+1$.

Data collection: *CrysAlis PRO* (Agilent, 2013); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008) within *OLEX2* (Dolomanov *et al.*, 2009); molecular graphics: *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* and *PLATON*.

Supporting information for this paper is available from the IUCr electronic archives (Reference: GK2601).

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# supporting information

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## Fluoren-9-one oxime

**Bernhard Bugenhagen, Yosef Al Jasem, Mariam Al-Azani and Thies Thiemann**

### S1. Comment

The title compound, which was prepared according to a known procedure (Moore & Huntress, 1927) has found extensive use as a starting material for preparation of medicinal active compounds such as novel cyclophilin A inhibitors (Ni *et al.*, 2009), novel analogs of beta-adrenoceptor antagonists (Rad *et al.*, 2012) and beta-blocker (Amlaiky *et al.*, 1983).

The ring atoms, N and O atoms in the title compound molecule, are essentially coplanar with a maximum deviation of 0.079 (2) Å for the O atom from the averaged ring plane (13 carbon atoms). The molecule in the crystal exhibits a C12—H12···O1 intramolecular interaction (Table 1), (Figure 1). The molecules related by a twofold screw axis are connected by O1—H1···N1 hydrogen bonds (Table 1) within a helical bonding network extending along the *a* axis (Figure 2). Within one helical bonding network, the neighboring molecules related by a unit translation along [100] show $\pi$–$\pi$ stacking interactions between their fluorene ring systems with the interplanar distance of 3.347 (2) Å (Figure 2). The neighboring helical bonding networks in parallel alignment are linked to each other by C5—H5··· $\pi$ (*Cg*1) (Table 1) close contact between their fluorene groups (Figure 3). The dihedral angle between the fluorene units of adjacent molecules along the helix is 88.40 (2)°.

### S2. Experimental

To a solution of fluoren-9-one (1.8 g, 10 mmol) in EtOH (47 ml) was given a solution of hydroxylamine hydrochloride ($NH_2OH{\cdot}HCl$, 2.75 g, 39.6 mmol) in water (7 ml), and the resulting mixture was stirred at 70 °C for 5 h. Thereafter, the reaction mixture was cooled and given into water (150 ml). The colorless precipitate was extracted with $CH_2Cl_2$ (2 × 75 ml). The organic phase was dried over anhydrous $MgSO_4$ and concentrated *in vacuo* to give fluoren-9-one oxime (1.79 g, 92%) as a colorless solid, mp. 471 – 472 K; $\nu_{max}$ (KBr/cm$^{-1}$) 3500 – 2800 (bs, OH), 1604 (w), 1602, 1450, 1405, 1317, 1156, 1089, 998, 937, 780, 732, 640; $\delta_H$ (400 MHz, $CDCl_3$) 7.28 – 7.47 (4*H*, m), 7.62 (1*H*, d, $^3J$ = 7.6 Hz), 7.66 (1*H*, d, $^3J$ = 7.2 Hz), 7.77 (1*H*, d, $^3J$ = 7.2 Hz), 8.42 (1*H*, d, $^3J$ = 7.6 Hz); $\delta_C$ (100.5 MHz, $CDCl_3$) 119.8 (CH), 119.9 (CH), 121.7 (CH), 128.0 (CH), 128.4 (CH), 129.7 (CH), 130.2 (CH), 130.3 ($C_{quat}$), 131.3 (CH), 135.1 ($C_{quat}$), 140.5 ($C_{quat}$), 141.4 ($C_{quat}$), 153.6 ($C_{quat}$). Single crystals were obtained from cold $CH_2Cl_2$.

### S3. Refinement

All carbon-bound hydrogen atoms, except the H of the OH group which was freely refined, were placed in calculated positions with C—H distance of 0.95 Å and refined as riding with *Uiso*(H) = 1.2*Ueq*(C).

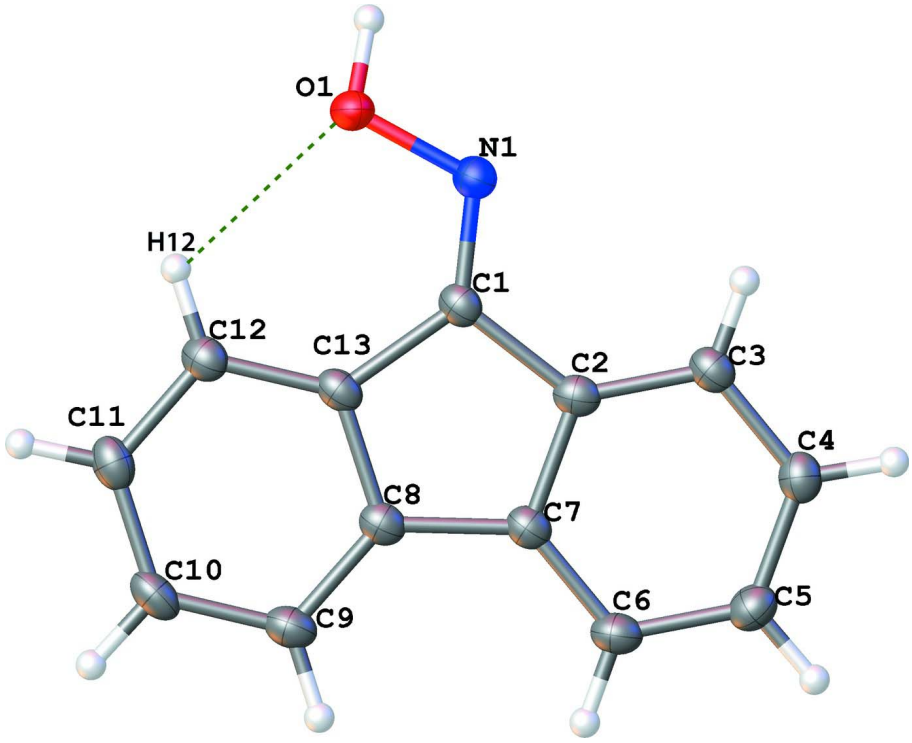


**Figure 1**

A view of the title molecule with displacement ellipsoids shown at the 50% probability level, showing the intramolecular contact within the molecule.

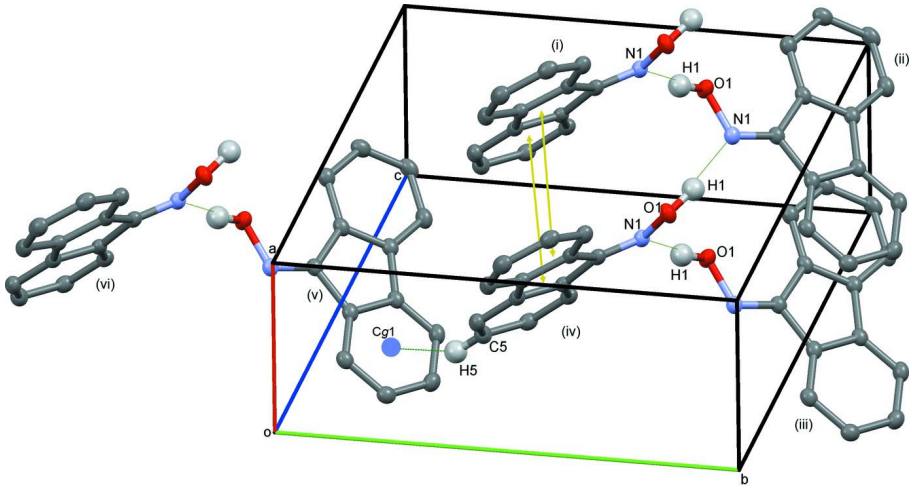


**Figure 2**

Intermolecular interactions between molecules of the title compound, including the $\pi$–$\pi$ stacking interactions (represented by arrows in yellow). [Symmetry codes: i: 1 + *x*,*y*,*z*; ii: 1/2 + *x*,1.5 - *y*,1 - *z*; iii: -1/2 + *x*,1.5 - *y*,1 - *z*; iv: *x*, *y*, *z*; v: -1/2 + *x*, 1/2 - *y*, 1 - *z*; vi: *x*, -1 + *y*, *z*]

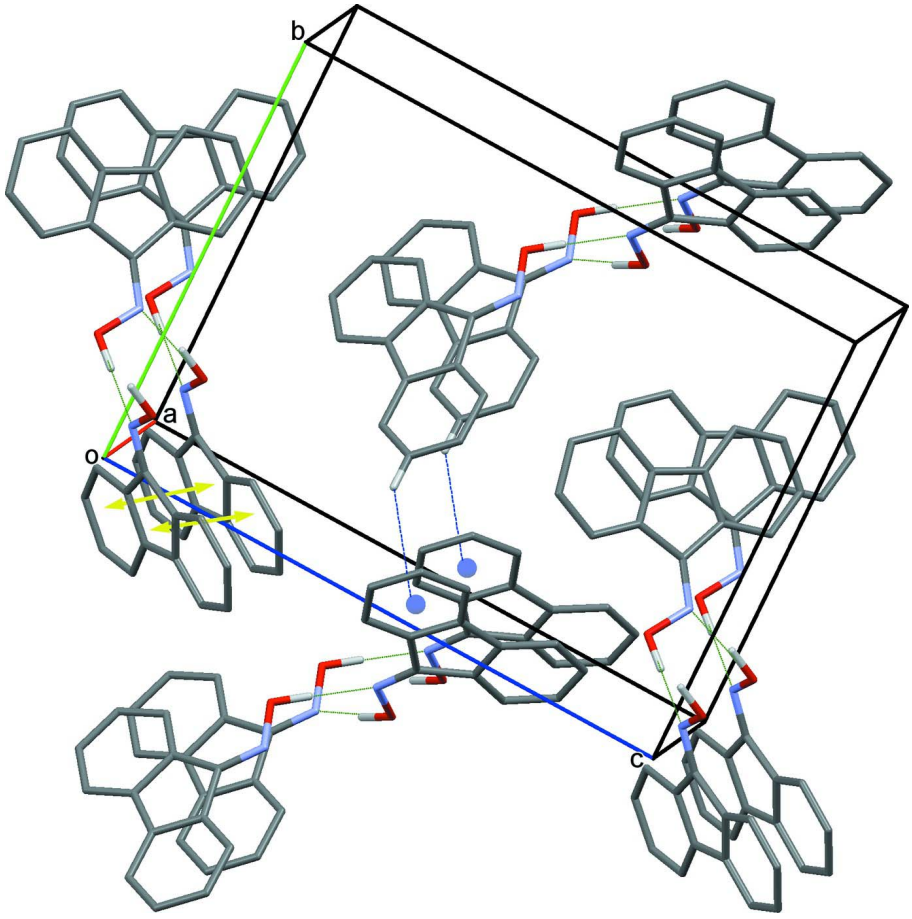


**Figure 3**

The crystal packing diagram showing the O—H···N close contacts (colored in green) between adjacent molecules in each helical bonding network, C—H···$\pi$ intermolecular interaction between molecules within different helices (colored in blue) and $\pi$–$\pi$ stacking interactions (arrows in yellow).

## Fluoren-9-one oxime

*Crystal data*

$C_{13}H_9NO$
$M_r$ = 195.21
Orthorhombic, $P2_12_12_1$
$a$ = 4.8009 (1) Å
$b$ = 12.2309 (2) Å
$c$ = 16.0247 (3) Å
$V$ = 940.96 (3) Å$^3$
$Z$ = 4
$F$(000) = 408

$D_x$ = 1.378 Mg m$^{-3}$
Melting point = 471–472 K
Cu $K\alpha$ radiation, $\lambda$ = 1.5418 Å
Cell parameters from 3850 reflections
$\theta$ = 4.5–76.1°
$\mu$ = 0.70 mm$^{-1}$
$T$ = 100 K
Block, colourless
0.16 × 0.13 × 0.13 mm

*Data collection*

Agilent SuperNova (Dual, Cu at zero, Atlas) diffractometer
Radiation source: SuperNova (Cu) X-ray Source

Mirror monochromator
Detector resolution: 10.4127 pixels mm$^{-1}$
$\omega$ scans

Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2013)
$T_{min}$ = 0.890, $T_{max}$ = 1.000
7588 measured reflections
1942 independent reflections
1865 reflections with $I > 2\sigma(I)$

$R_{int}$ = 0.029
$\theta_{max}$ = 76.3°, $\theta_{min}$ = 4.6°
$h$ = −6→5
$k$ = −14→15
$l$ = −19→20

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.075
$S$ = 1.05
1942 reflections
140 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: difference Fourier map

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0384P)^2 + 0.1723P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$
Absolute structure: Flack parameter determined using 735 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.16 (13)

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.5506 (4) | 0.58330 (13) | 0.40422 (10) | 0.0189 (4) |
| C10 | 0.8197 (4) | 0.44386 (15) | 0.17647 (10) | 0.0251 (4) |
| C11 | 0.9543 (4) | 0.53953 (15) | 0.20052 (10) | 0.0242 (4) |
| C12 | 0.8830 (4) | 0.59306 (14) | 0.27456 (10) | 0.0219 (4) |
| C13 | 0.6741 (4) | 0.54803 (13) | 0.32367 (10) | 0.0196 (3) |
| C2 | 0.3367 (4) | 0.50126 (13) | 0.42679 (10) | 0.0194 (3) |
| C3 | 0.1613 (4) | 0.49391 (13) | 0.49503 (10) | 0.0209 (3) |
| C4 | −0.0178 (4) | 0.40413 (13) | 0.50050 (11) | 0.0228 (4) |
| C5 | −0.0177 (4) | 0.32387 (14) | 0.43891 (11) | 0.0246 (4) |
| C6 | 0.1590 (4) | 0.33133 (14) | 0.37017 (11) | 0.0235 (4) |
| C7 | 0.3353 (4) | 0.42037 (13) | 0.36414 (10) | 0.0195 (3) |
| C8 | 0.5403 (4) | 0.45037 (13) | 0.30001 (10) | 0.0198 (4) |
| C9 | 0.6112 (4) | 0.39797 (14) | 0.22607 (11) | 0.0239 (4) |
| H1 | 0.898 (6) | 0.773 (2) | 0.4668 (17) | 0.068 (9)* |
| H10 | 0.8703 | 0.4093 | 0.1256 | 0.030* |
| H11 | 1.0969 | 0.5689 | 0.1661 | 0.029* |
| H12 | 0.9750 | 0.6584 | 0.2908 | 0.026* |
| H3 | 0.1626 | 0.5485 | 0.5372 | 0.025* |
| H4 | −0.1408 | 0.3978 | 0.5467 | 0.027* |
| H5 | −0.1399 | 0.2631 | 0.4438 | 0.029* |
| H6 | 0.1583 | 0.2764 | 0.3283 | 0.028* |
| H9 | 0.5200 | 0.3325 | 0.2097 | 0.029* |

| | | | | |
|---|---|---|---|---|
| N1 | 0.6059 (3) | 0.66488 (11) | 0.45230 (8) | 0.0202 (3) |
| O1 | 0.8178 (3) | 0.73127 (10) | 0.42014 (7) | 0.0233 (3) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0217 (9) | 0.0194 (8) | 0.0158 (7) | 0.0029 (6) | −0.0016 (6) | 0.0013 (6) |
| C10 | 0.0300 (10) | 0.0290 (8) | 0.0164 (7) | 0.0078 (8) | −0.0003 (7) | −0.0031 (7) |
| C11 | 0.0257 (9) | 0.0289 (9) | 0.0179 (8) | 0.0060 (7) | 0.0018 (7) | 0.0038 (7) |
| C12 | 0.0266 (9) | 0.0206 (7) | 0.0186 (8) | 0.0025 (7) | −0.0013 (7) | 0.0015 (6) |
| C13 | 0.0228 (9) | 0.0204 (7) | 0.0155 (7) | 0.0050 (7) | −0.0024 (7) | −0.0007 (6) |
| C2 | 0.0216 (8) | 0.0185 (7) | 0.0181 (8) | 0.0028 (7) | −0.0048 (7) | 0.0005 (6) |
| C3 | 0.0233 (8) | 0.0219 (7) | 0.0174 (7) | 0.0043 (7) | −0.0018 (7) | 0.0005 (6) |
| C4 | 0.0223 (8) | 0.0248 (8) | 0.0214 (8) | 0.0028 (6) | 0.0007 (8) | 0.0042 (7) |
| C5 | 0.0259 (9) | 0.0210 (8) | 0.0268 (9) | −0.0024 (7) | −0.0015 (7) | 0.0030 (7) |
| C6 | 0.0277 (10) | 0.0200 (7) | 0.0228 (8) | 0.0012 (7) | −0.0040 (7) | −0.0025 (6) |
| C7 | 0.0209 (8) | 0.0200 (7) | 0.0177 (7) | 0.0037 (6) | −0.0021 (6) | −0.0002 (6) |
| C8 | 0.0212 (9) | 0.0202 (7) | 0.0181 (8) | 0.0034 (7) | −0.0032 (7) | −0.0001 (6) |
| C9 | 0.0287 (10) | 0.0220 (8) | 0.0209 (8) | 0.0030 (7) | −0.0039 (7) | −0.0034 (6) |
| N1 | 0.0236 (8) | 0.0184 (6) | 0.0185 (7) | 0.0010 (6) | −0.0008 (6) | 0.0014 (5) |
| O1 | 0.0283 (6) | 0.0217 (5) | 0.0198 (6) | −0.0058 (5) | 0.0010 (5) | −0.0023 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C13 | 1.484 (2) | C4—H4 | 0.9500 |
| C1—C2 | 1.481 (2) | C5—C6 | 1.393 (2) |
| C10—C11 | 1.391 (3) | C5—H5 | 0.9500 |
| C10—H10 | 0.9500 | C6—C7 | 1.383 (2) |
| C11—C12 | 1.398 (2) | C6—H6 | 0.9500 |
| C11—H11 | 0.9500 | C7—C8 | 1.469 (2) |
| C12—C13 | 1.389 (2) | C8—C13 | 1.408 (2) |
| C12—H12 | 0.9500 | C8—C9 | 1.389 (2) |
| C2—C7 | 1.410 (2) | C9—C10 | 1.396 (3) |
| C2—C3 | 1.383 (2) | C9—H9 | 0.9500 |
| C3—C4 | 1.397 (2) | N1—C1 | 1.288 (2) |
| C3—H3 | 0.9500 | O1—H1 | 0.98 (3) |
| C4—C5 | 1.392 (2) | O1—N1 | 1.4000 (19) |
| | | | |
| N1—O1—H1 | 107.7 (17) | C6—C7—C2 | 120.39 (16) |
| C1—N1—O1 | 112.25 (13) | C6—C7—C8 | 130.96 (16) |
| N1—C1—C2 | 121.43 (15) | C9—C8—C7 | 130.19 (16) |
| N1—C1—C13 | 131.53 (16) | C9—C8—C13 | 120.61 (16) |
| C2—C1—C13 | 107.00 (14) | C13—C8—C7 | 109.20 (14) |
| C3—C2—C1 | 131.26 (15) | C8—C9—H9 | 120.8 |
| C3—C2—C7 | 120.97 (15) | C8—C9—C10 | 118.41 (16) |
| C7—C2—C1 | 107.75 (14) | C10—C9—H9 | 120.8 |
| C2—C3—H3 | 120.8 | C9—C10—H10 | 119.6 |
| C2—C3—C4 | 118.38 (15) | C11—C10—C9 | 120.89 (16) |

| | | | |
|---|---|---|---|
| C4—C3—H3 | 120.8 | C11—C10—H10 | 119.6 |
| C3—C4—H4 | 119.7 | C10—C11—H11 | 119.5 |
| C5—C4—C3 | 120.63 (16) | C10—C11—C12 | 121.04 (17) |
| C5—C4—H4 | 119.7 | C12—C11—H11 | 119.5 |
| C4—C5—H5 | 119.5 | C11—C12—H12 | 120.9 |
| C4—C5—C6 | 120.97 (17) | C13—C12—C11 | 118.17 (17) |
| C6—C5—H5 | 119.5 | C13—C12—H12 | 120.9 |
| C5—C6—H6 | 120.7 | C8—C13—C1 | 107.38 (15) |
| C7—C6—C5 | 118.66 (16) | C12—C13—C1 | 131.75 (16) |
| C7—C6—H6 | 120.7 | C12—C13—C8 | 120.87 (15) |
| C2—C7—C8 | 108.64 (14) | | |

| | | | |
|---|---|---|---|
| O1—N1—C1—C2 | 178.85 (14) | C5—C6—C7—C2 | 0.5 (3) |
| O1—N1—C1—C13 | 1.2 (2) | C5—C6—C7—C8 | −179.68 (17) |
| N1—C1—C2—C3 | 1.5 (3) | C6—C7—C8—C9 | 1.3 (3) |
| N1—C1—C2—C7 | −177.14 (15) | C6—C7—C8—C13 | −178.35 (18) |
| N1—C1—C13—C8 | 177.82 (17) | C7—C2—C3—C4 | 0.0 (2) |
| N1—C1—C13—C12 | −1.4 (3) | C7—C8—C9—C10 | −178.93 (17) |
| C1—C2—C3—C4 | −178.52 (16) | C7—C8—C13—C1 | −0.88 (18) |
| C1—C2—C7—C6 | 178.38 (15) | C7—C8—C13—C12 | 178.46 (15) |
| C1—C2—C7—C8 | −1.52 (18) | C8—C9—C10—C11 | 0.3 (3) |
| C2—C1—C13—C8 | −0.04 (18) | C9—C8—C13—C1 | 179.46 (15) |
| C2—C1—C13—C12 | −179.28 (17) | C9—C8—C13—C12 | −1.2 (2) |
| C2—C3—C4—C5 | 0.4 (2) | C9—C10—C11—C12 | −0.6 (3) |
| C2—C7—C8—C9 | −178.86 (18) | C10—C11—C12—C13 | 0.1 (3) |
| C2—C7—C8—C13 | 1.53 (18) | C11—C12—C13—C1 | 179.97 (17) |
| C3—C2—C7—C6 | −0.5 (2) | C11—C12—C13—C8 | 0.8 (2) |
| C3—C2—C7—C8 | 179.64 (15) | C13—C1—C2—C3 | 179.66 (16) |
| C3—C4—C5—C6 | −0.4 (3) | C13—C1—C2—C7 | 0.98 (18) |
| C4—C5—C6—C7 | 0.0 (3) | C13—C8—C9—C10 | 0.6 (2) |

*Hydrogen-bond geometry (Å, º)*

Cg1 is the centroid of the C2–C7 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C12—H12···O1 | 0.95 | 2.38 | 2.898 (2) | 114 |
| O1—H1···N1$^{i}$ | 0.98 (3) | 1.80 (3) | 2.7758 (18) | 169 (3) |
| C5—H5···*Cg*1$^{ii}$ | 0.95 | 3.08 | 3.873 | 142 |

Symmetry codes: (i) *x*+1/2, −*y*+3/2, −*z*+1; (ii) *x*−1/2, −*y*+1/2, −*z*+1.